

## A COUPLED MULTIPHASE-FIELD AND CARBON DIFFUSION MODEL FOR LOWER BAINITIC TRANSFORMATION

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**Abstract.** A multiphase-field method coupled to a Cahn-Hilliard diffusion model is presented in this paper. The underlying thermodynamic framework is based on the concept of generalized stresses. A prototype model is developed to simulate the lower bainitic transformation, including phase transitions, the separation of carbon within the supersaturated phase and the precipitation of carbides. The system of partial differential equations is solved with the finite element method. Numerical results of the model showing the qualitative mechanism are discussed.

### 1 INTRODUCTION

In this work the phase-field method is utilized to simulate the lower bainitic transformation, which is one of the most complex transformations in steel. The growth of the bainitic ferrite is assumed to be displacive [1] in contrast to the perlitic transformation which is highly dependent on the carbon diffusion and therefore is ranked as a diffusive transformation. The diffusion of carbon is a major mechanism of the bainitic transformation, too, since the precipitation of carbides from within the supersaturated bainitic ferrite is strongly dependent on the local carbon concentration. The displacive transformation from austenite to bainitic ferrite leads to a supersaturated phase. Within the bainitic ferrite the carbon separates and builds accumulations which precipitate as carbides [1].

To model this material behaviour a system of partial differential equations is developed, based on a thermodynamic framework of generalized stresses as introduced by Gurtin and Fried [2, 3] for a two phase Ginzburg-Landau system and a Cahn-Hilliard equation. We extend this framework for a viscous Cahn-Hilliard equation coupled to multiphase-field models [4] as it is needed for the lower bainitic transformation. The key aspects of the

thermodynamic framework are generalized stresses and microforces which perform work in conjunction with derivatives of the phase-field variables and the carbon concentration. The framework distinguishes between basic balance laws which are universal and constitutive equations which depend on the specific material. The Clausius-Duhem inequality is used to impose restrictions to the constitutive equations. The numerical examples show the qualitative mechanism of the lower bainitic transformation as discussed above.

## 2 THERMODYNAMIC FRAMEWORK

The thermodynamic framework is based on the microforce balance as introduced by Gurtin and Fried [2, 3] and generalized by Ammar et al. [5]. Thereby, an extended version as described in [4] and [6] is used to combine a multiphase Ginzburg-Landau equation for the phase-field problem coupled with a Cahn-Hilliard diffusion equation. The carbon concentration is identified by  $c$  and the phase order parameters are labelled  $\phi_i$ .

For  $N_p$  phases we start by defining  $N_p$  *vector phase stresses*  $\vec{\xi}_i$ , *internal scalar phase forces*  $\pi_i$  and *external scalar phase forces*  $\gamma_i$  over the volume  $B$ . The power performed on the atomic configurations within a region  $V$  of  $B$  for each phase  $i$  reads

$$\int_V -\vec{\xi}_i \cdot \nabla \dot{\phi}_i dV, \quad \int_V \pi_i \dot{\phi}_i dV, \quad \int_V \gamma_i \dot{\phi}_i dV, \quad i = 1, \dots, N_p. \quad (1)$$

A similar definition is needed for the Cahn-Hilliard equation where  $\omega$  is introduced as a *scalar internal diffusion force* and  $\vec{\lambda}$  as a *vector diffusion stress*. The powers are

$$\int_V -\vec{\lambda} \cdot \nabla \dot{c} dV, \quad \int_V \omega \dot{c} dV. \quad (2)$$

The system of microforces and microstresses in equations (1) and (2) shall be consistent with the microforce balance for each control volume  $V$

$$\sum_{i=1}^{N_p} \left( - \int_V \vec{\xi}_i \cdot \nabla \dot{\phi}_i dV + \int_V \pi_i \dot{\phi}_i dV + \int_V \gamma_i \dot{\phi}_i dV \right) - \int_V \vec{\lambda} \cdot \nabla \dot{c} dV + \int_V \omega \dot{c} dV = 0 \quad (3)$$

which leads to the *local microforce balances*

$$\nabla \cdot \vec{\xi}_i + \pi_i + \gamma_i = 0 \quad \text{in } V \quad \text{for } i = 1, \dots, N_p, \quad (4)$$

$$\nabla \cdot \vec{\lambda} + \omega = 0 \quad \text{in } V, \quad (5)$$

$$\vec{\xi}_i \cdot \vec{n} = 0 \quad \text{on } \partial V \quad \text{for } i = 1, \dots, N_p, \quad (6)$$

$$\vec{\lambda} \cdot \vec{n} = 0 \quad \text{on } \partial V. \quad (7)$$

In the isothermal case, which is analyzed here, the *local dissipation inequality*

$$-\dot{\psi} + \vec{\lambda} \cdot \nabla \dot{c} - \omega \dot{c} + \mu \dot{c} - \vec{J} \cdot \nabla \mu + \sum_{i=1}^{N_p} \left( \vec{\xi}_i \cdot \nabla \dot{\phi}_i - \pi_i \dot{\phi}_i \right) \geq 0. \quad (8)$$

can be formulated using mass conservation, the first and the second law of thermodynamics [4], where  $\psi$  is the Helmholtz energy,  $\mu$  the chemical potential and  $\vec{J}$  the flux.

In a next step restrictions to constitutive equations can be formulated with the help of the local dissipation inequality (8). After some transformation (for details see [4]) the dissipation inequality reads

$$\mathcal{D} = \nabla\mu \cdot \mathbf{A}\nabla\mu + \tau\dot{c}^2 + \sum_{i=1}^{N_p} \beta_i \dot{\phi}_i^2 \geq 0, \quad (9)$$

where  $\mathbf{A}$  is a mobility tensor and  $\tau$  and  $\beta_i$  are constitutive moduli. It turns out that the inequality (9) holds for any choice of  $\nabla\mu, \dot{c}$  and  $\dot{\phi}_i$  if and only if

$$\tau \geq 0, \quad \beta_i \geq 0, \quad \vec{s} \cdot \mathbf{A}\vec{s} \geq 0 \quad \forall \vec{s}. \quad (10)$$

### 3 PROTOTYPE MODEL FOR LOWER BAINITE

#### 3.1 Evolution equations

In this prototype model for lower bainite the evolution of 3 phases, namely bainitic ferrite ( $\phi_1$ ), austenite ( $\phi_2$ ) and carbide ( $\phi_3$ ) is described in parallel with the diffusion of carbon which is strongly coupled to the phase growth. Choosing constitutive equations for the Helmholtz energy  $\psi$ , the constitutive moduli  $\tau$  and  $\beta_i$  and the mobility tensor  $\mathbf{A}$  to describe the growth kinetics of lower bainite under consideration of the restrictions (10), we finally end up with an evolution equation for the diffusion

$$\dot{c} = \phi_1 \kappa \Delta \left( \frac{\partial f(c)}{\partial c} - \rho \Delta c + \tau \dot{c} \right) + \nabla \phi_1 \kappa \nabla \left( \frac{\partial f(c)}{\partial c} - \rho \Delta c + \tau \dot{c} \right), \quad (11)$$

where  $\kappa$  is the diffusion coefficient,  $\rho$  the balance factor and  $f$  the carbon potential function.

Changing parameters as described in [7] and [8] leads to an evolution equation for the multiphase-field with the physical material parameters, interface mobilities  $\zeta_{ij}$ , interface energies  $\sigma_{ij}$ , interface thicknesses  $\eta_{ij}$  and Gibbs energy  $\Delta G_{ij}$

$$\dot{\phi}_i = \sum_{j=1, j \neq i}^{N_p} \zeta_{ij} \left[ \sigma_{ij} \left( (\phi_j \Delta \phi_i - \phi_i \Delta \phi_j) - \frac{36}{\eta_{ij}^2} \phi_i \phi_j (\phi_j - \phi_i) \right) - \frac{6 \cdot \Delta G_{ij}}{\eta_{ij}} \phi_i \phi_j \right] \quad \text{for } i = 1, \dots, N_p. \quad (12)$$

#### 3.2 Carbide precipitation

A main mechanism of the lower bainitic transformation is the precipitation of carbides, because the small carbides influence the macroscopic material behavior significantly. The simulation of the precipitation process yields several challenges. The phase-field method

(12) is not able to simulate the growth of a phase  $\phi_i$  whose value is zero over the whole domain. Therefore, small nuclei of carbides are defined as initial conditions. However in this special case the nuclei nearly vanish while the austenite transforms into ferrite and cannot grow any more. An elegant way to solve this problem and model the physical precipitation of carbides is to define the thermodynamic driving force as a constitutive equation as follows:

$$\Delta G_{ij}(\vec{z}) = \Delta G_{ij}^0 v(\phi_i, \phi_j, c) \quad (13)$$

where

$$v(\phi_i, \phi_j, c) = \begin{cases} \frac{w(c)}{\phi_3^2} & \text{for } i = 3 \vee j = 3 \\ 1 & \text{otherwise} \end{cases} \quad (14)$$

and  $\Delta G_{ij}^0$  is a constant material parameter. The function  $w(c)$  is a smooth unit step function

$$w(c) = \begin{cases} 0 & \text{for } c < c_{\text{carb}} - \varepsilon \\ 1 & \text{for } c > c_{\text{carb}} \\ \frac{1}{2} + \frac{1}{2} \cdot \sin\left(\frac{\pi}{\varepsilon} \cdot c + \frac{\pi}{2} - \frac{\pi}{\varepsilon} \cdot c_{\text{carb}}\right) & \text{otherwise,} \end{cases} \quad (15)$$

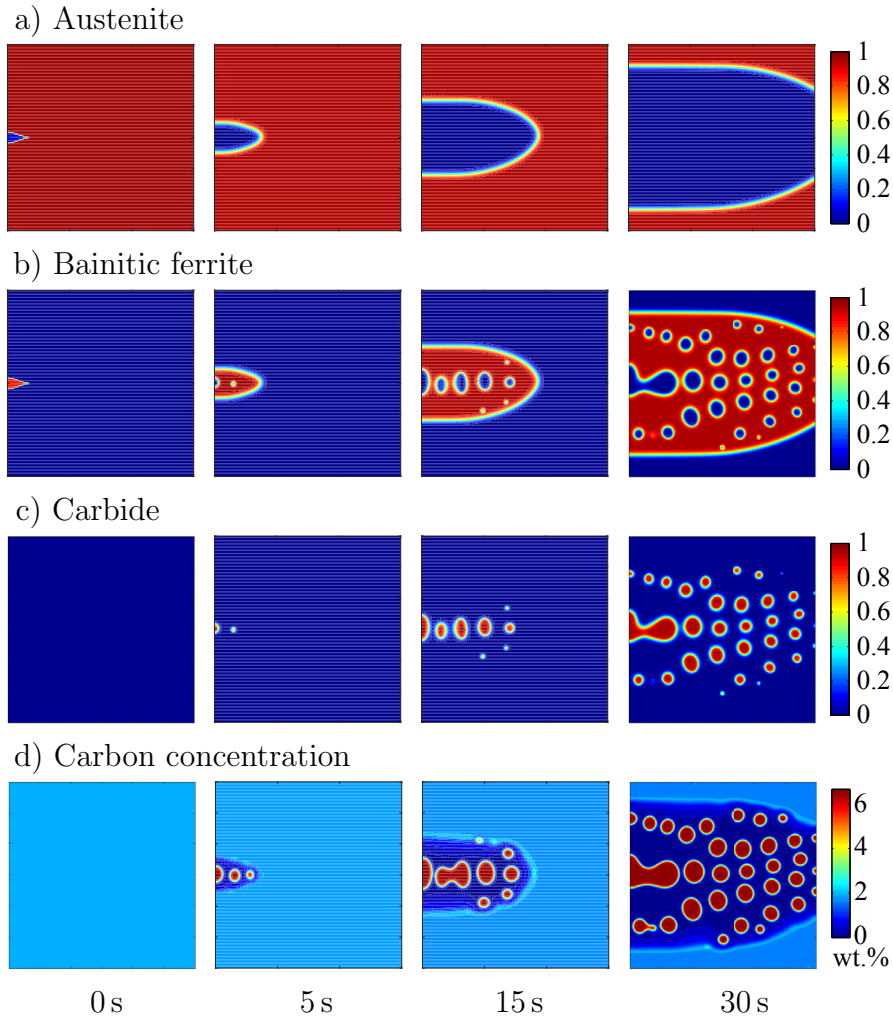
where the parameter  $\varepsilon$  governs the width of the transition zone and  $c_{\text{carb}}$  specifies the maximum carbon concentration.

The Gibbs energy formulation (13) - (15) does not change the transformation kinetics between austenite ( $\phi_2$ ) and bainitic ferrite ( $\phi_1$ ). Only in case of high carbon concentration at a certain place the carbide phase ( $\phi_3$ ) will grow due to equations (14) and (15). The function  $v$  ensures that the carbide phase can grow even if the nuclei have become very small in time.

#### 4 IMPLEMENTATION AND NUMERICAL EXAMPLE

Numerical solutions for the coupled evolution equations (11) and (12) are obtained with the finite element method in two dimensions. Here the partial differential equations are discretized over an domain of  $3\mu\text{m} \times 3\mu\text{m}$  with quadrilateral elements and linear shape functions. The fine mesh has about 16384 elements. For the time discretization an implicit Euler scheme is implemented. Here we used a time step of 0.05s and compute solutions until 30s.

Figure 1 shows representative results of the numerical example. In the first row (a) the austenite phase is shown, in the second the row (b) one can see the bainitic ferrite phase. In Figure 1.c) the carbides are shown. All three phases vary between 0 and 1, where 0 means that the phase is not present at that local point and 1 means that only this phase is present here. The sum of all three phases is one at every local point. The columns in



**Figure 1:** Lower bainitic transformation after 0s, 5s, 15s and 30s.

Figure 1 represent the results of the four fields after 0s, 5s, 15s and 30s. The first column shows the initial conditions. There is a small nucleus of bainitic ferrite at the right border of the domain. There are no carbides at the beginning and the carbon concentration is uniformly distributed over the whole domain. In fact there are small perturbations of carbon and small initial nuclei of carbides randomly distributed. After 5s the bainitic ferrite sheaf has grown and as shown in Figure 1.d) the carbon within the supersaturated bainitic ferrite starts to separate and build accumulations of carbon. At points where the local carbon concentration reaches the maximum concentration  $c_{\text{carb}}$  carbides precipitate. In the next two time steps shown here, one can see the growing bainitic ferrite sheaf and the results of the Cahn-Hilliard diffusion equation. Several accumulations of carbon rise up and therefore carbides grow at this places.

## 5 CONCLUSIONS

A thermodynamic framework and a prototype model for lower bainite are presented in this work. The framework can be used for any kind of Cahn-Hilliard diffusion models coupled to multiphase-field methods. It is based on universal laws, such as mass conservation, energy conservation, the balance of microforces and the second law of thermodynamics, which are strictly separated from constitutive equations. The lower bainite model shows the described growth mechanisms, like the displacive transformation from austenite to bainitic ferrite, the separation of carbon within the supersaturated bainitic ferrite and the precipitation of carbides at carbon accumulations.

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